

# Structures: 1

> d his

(FILE 'REGISTRY' ENTERED AT 08:37:35 ON 19 MAR 2003)

L1 STR  
L2 0 S L1 } #22 st no anticipet.  
L3 0 S L1 FUL  
ACT WAL4AND11/A

L4 STR not main  
L5 ( 5)SEA FILE=REGISTRY SSS FUL L4 not main  
L6 STR #11 & 4 str  
L7 2 SEA FILE=REGISTRY SUB=L5 SSS FUL L6 }  
ACT WAL5AND10/A

L8 STR #5 & #10 } Structures #5 and #10 -  
L9 1 SEA FILE=REGISTRY SSS FUL L8 }  
ACT WAL8AND12/A

L10 STR #8 & 12  
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ACT WAL13/A

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ACT WAL15/A

L16 STR #15  
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ACT WAL17AND19/A

L18 STR  
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L20 STR → #10 & 17  
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ACT WAL21/A

L22 STR #21  
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L24 12 S L7 OR L9 OR L11 OR L15 OR L17 OR L21 OR L23

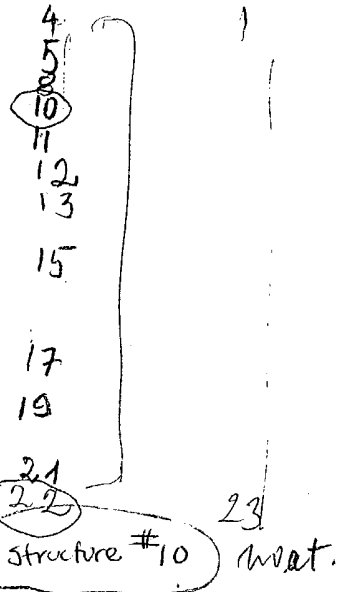
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L25 8 S L24

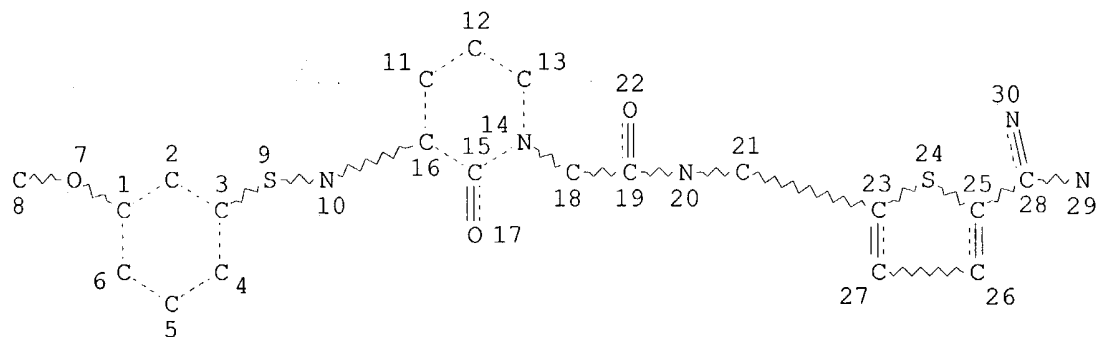
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FILE 'REGISTRY' ENTERED AT 10:05:11 ON 19 MAR 2003



=> d stat que 13  
L1 STR



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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 30

STEREO ATTRIBUTES: NONE  
L3 0 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 26 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

=&gt; fil hcaplus

FILE 'HCAPLUS' ENTERED AT 09:59:51 ON 19 MAR 2003

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FILE COVERS 1907 - 19 Mar 2003 VOL 138 ISS 12

FILE LAST UPDATED: 18 Mar 2003 (20030318/ED)

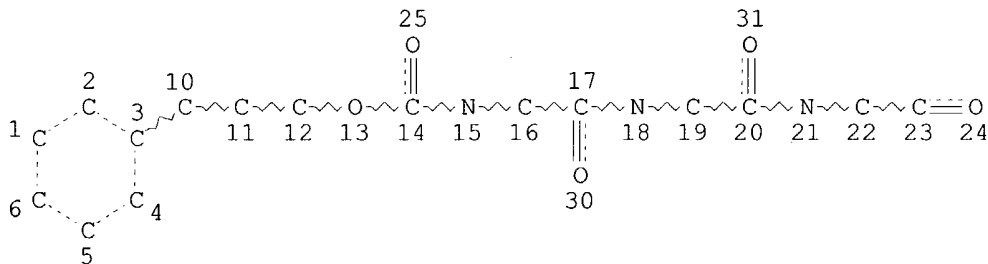
This file contains CAS Registry Numbers for easy and accurate substance identification.

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L4 STR



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DEFAULT ECLEVEL IS LIMITED

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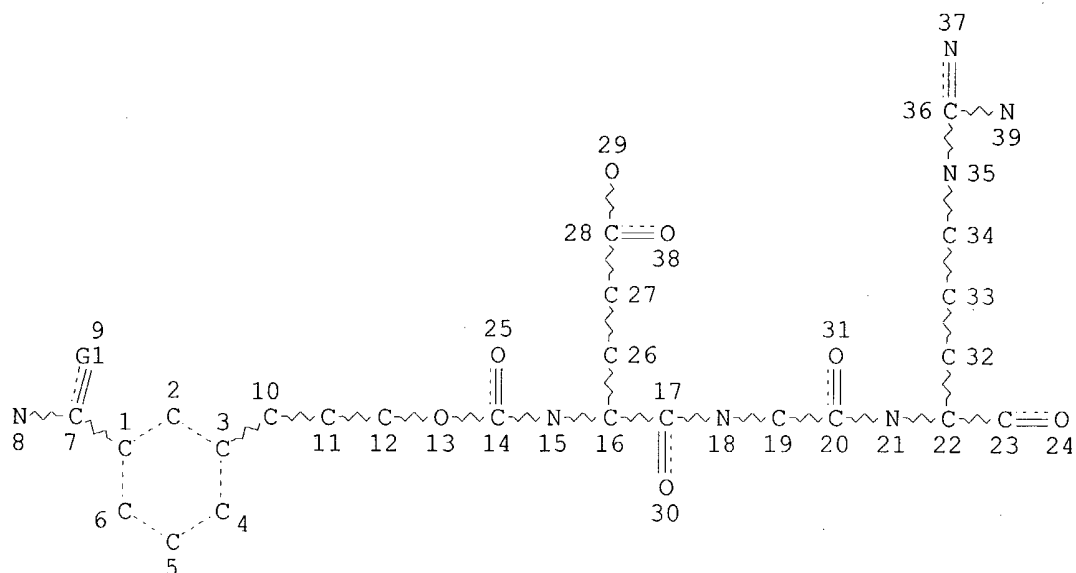
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VAR G1=O/N

NODE ATTRIBUTES:

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

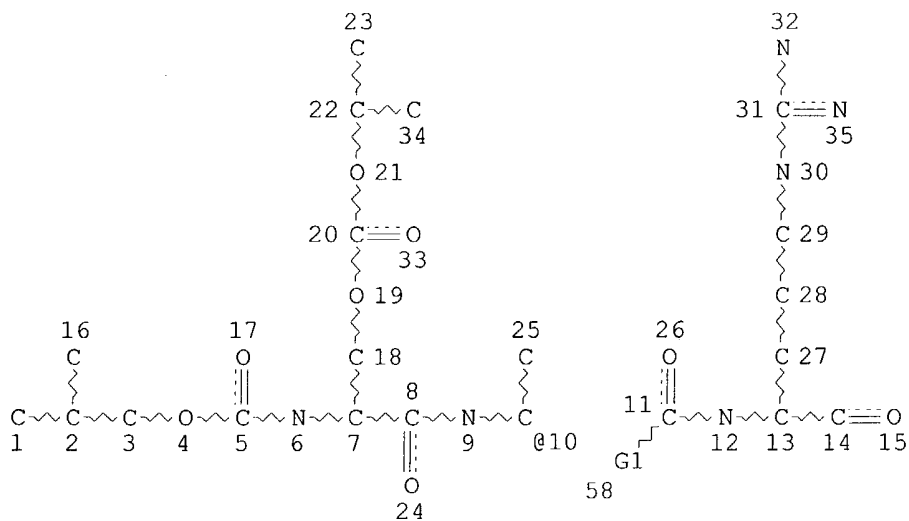
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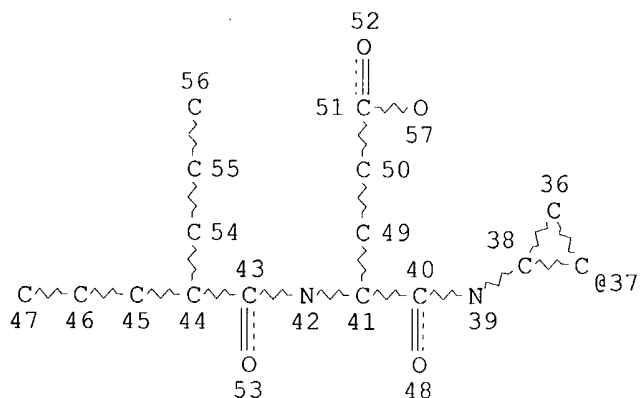
NUMBER OF NODES IS 39

STEREO ATTRIBUTES: NONE

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L8 STR





Page 4-A

VAR G1=10/37

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

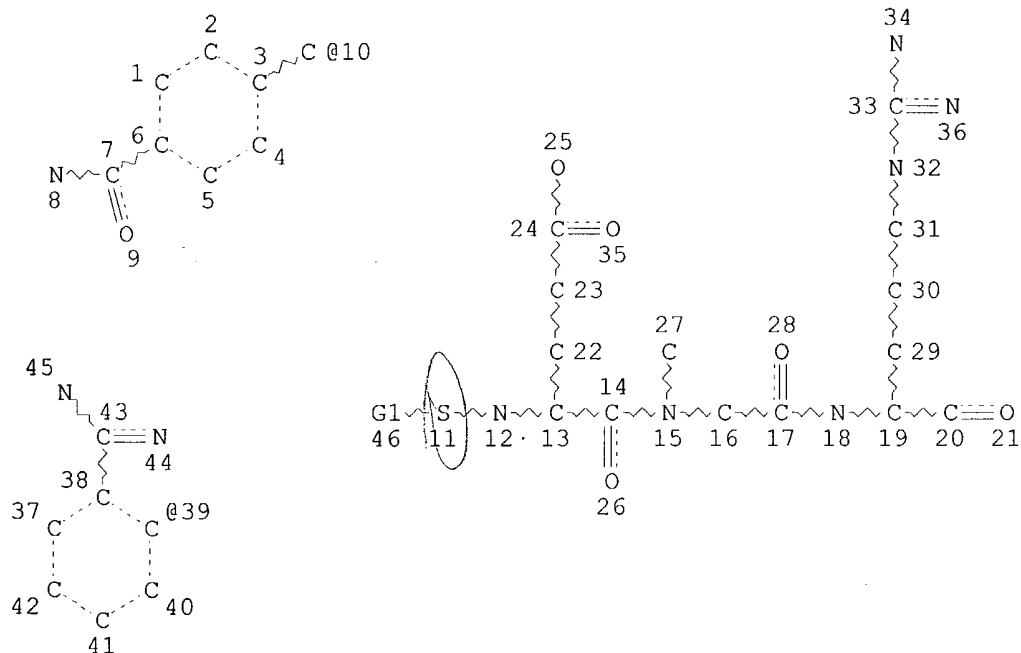
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STEREO ATTRIBUTES: NONE

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L10 STR



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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

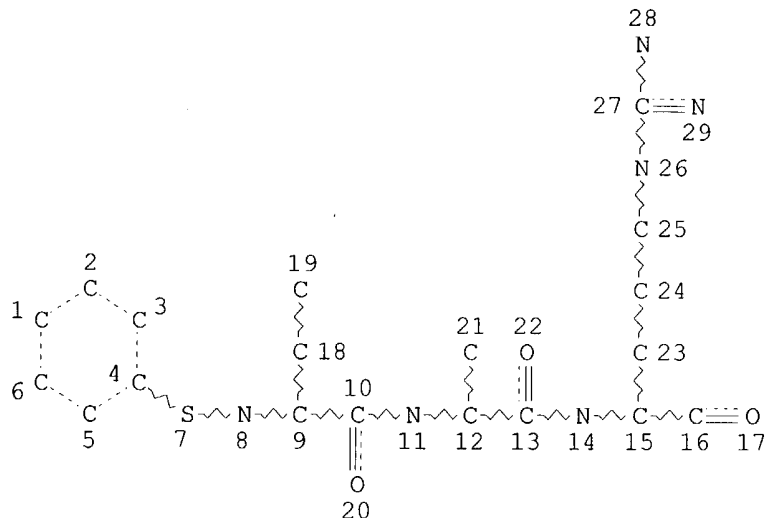
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L12 STR



NODE ATTRIBUTES:

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

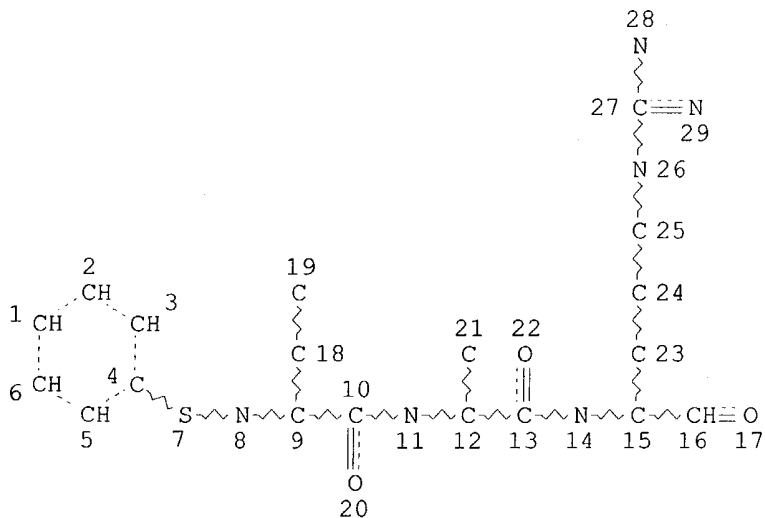
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NUMBER OF NODES IS 29

STEREO ATTRIBUTES: NONE

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L14 STR



NODE ATTRIBUTES:

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DEFAULT ECLEVEL IS LIMITED

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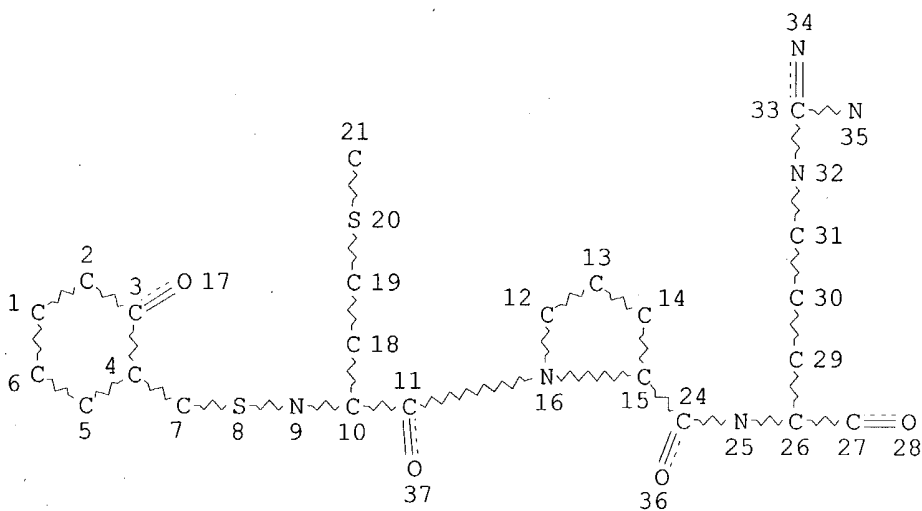
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NUMBER OF NODES IS 29

STEREO ATTRIBUTES: NONE

L15 1 SEA FILE=REGISTRY SUB=L13 SSS FUL L14

L16 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

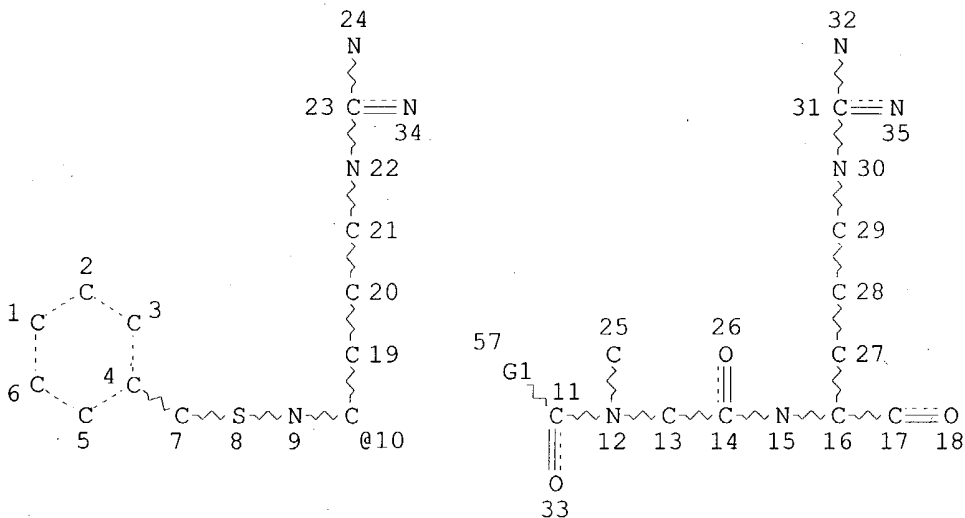
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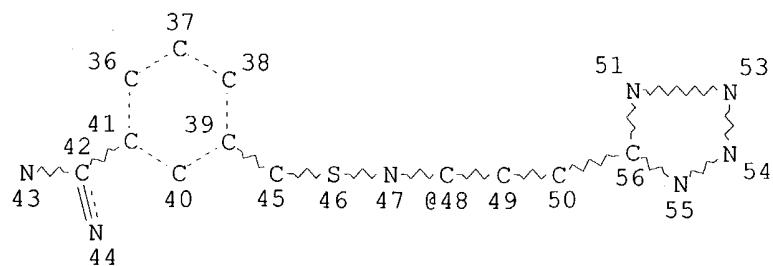
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STEREO ATTRIBUTES: NONE

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Page 2-A

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DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

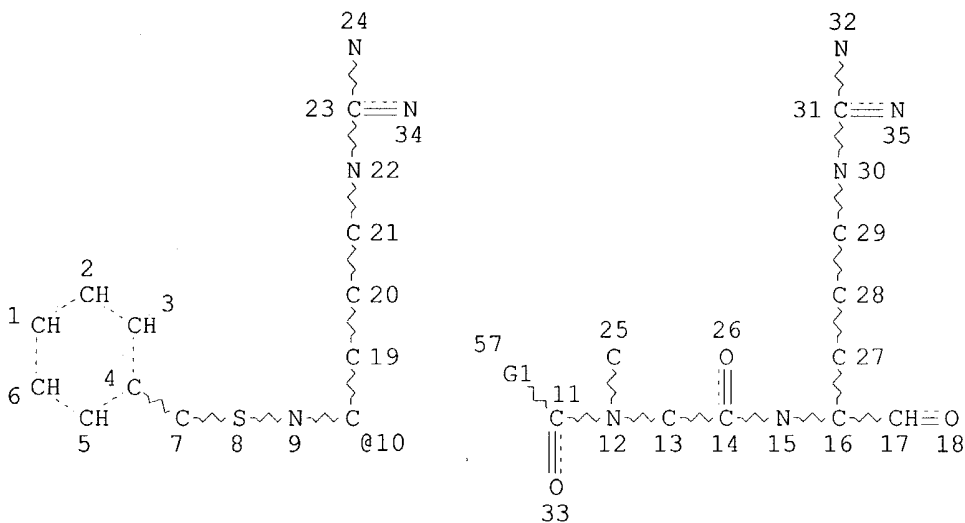
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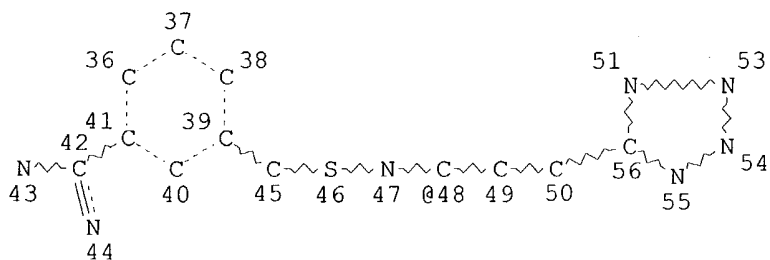
STEREO ATTRIBUTES: NONE

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L20 STR



Page 1-A



Page 2-A

VAR G1=10/48

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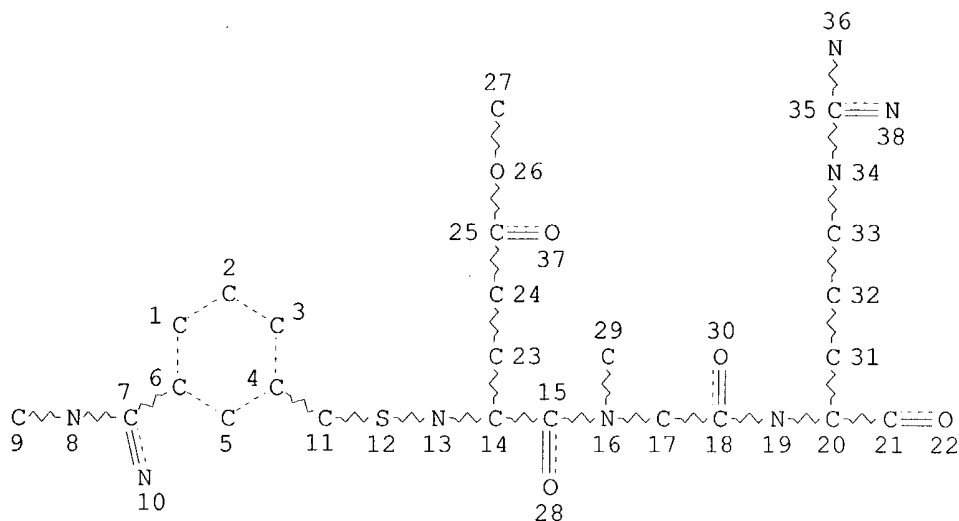


DEFAULT MLEVEL IS ATOM  
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GRAPH ATTRIBUTES:  
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 NUMBER OF NODES IS 56

STEREO ATTRIBUTES: NONE

L21 3 SEA FILE=REGISTRY SUB=L19 SSS FUL L20  
 L22 STR



NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 38

STEREO ATTRIBUTES: NONE

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 L24 12 SEA FILE=REGISTRY ABB=ON PLU=ON L7 OR L9 OR L11 OR L15 OR  
 L17 OR L21 OR L23  
 L25 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L24

=>  
 =>

=> d ibib abs hitrn l25 1-8

L25 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 2003:203392 HCAPLUS  
 TITLE: Preparation of peptides as inhibitors of serine  
 protease activity of matriptase or MTSP1  
 INVENTOR(S): Semple, Joseph E.; Coombs, Gary S.; Reiner, John E.;  
 Ong, Edgar O.; Araldi, Gian Luca  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 34 pp., Cont.-in-part of Appl.  
 No. PCT/US01/28137.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003050251	A1	20030313	US 2002-92004	20020305
WO 2002020475	A2	20020314	WO 2001-US28137	20010907

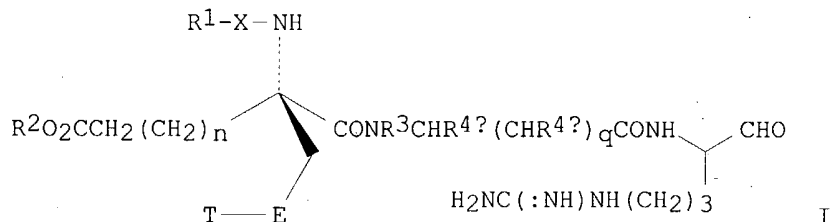
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

US 2000-657986 A2 20000908  
WO 2001-US28137 A2 20010907

GI



AB The invention provides compds. I [X = CO, CO<sub>2</sub>, CONH, SO<sub>2</sub>, SO<sub>2</sub>NH or a direct link; R<sub>1</sub> = (un)substituted alkyl, cycloalkyl, aryl, heterocycloalkyl, H when X is CONH, SO<sub>2</sub>, SO<sub>2</sub>NH or a direct link, etc.; R<sub>2</sub> = H, alkyl; n = 0-3; R<sub>3</sub> = H, Me; R<sub>4a</sub>, R<sub>4b</sub> = H, alkyl; q = 0-2; when q = 0, R<sub>3</sub> and R<sub>4a</sub> form prolyl or prolyl derivs., pipercolyl, or azetidine-2-carbonyl groups which are in the S-configuration; E is a 5- or 6-membered arom. ring having 0-2 ring heteroatoms; T is H, OH, CH<sub>2</sub>OH, alkyl, cyano, an amidino, guanidino, amino or carbamoyl deriv.] which inhibit serine protease activity of matriptase or MTSP1. Also provided are pharmaceutical compns. for treating conditions ameliorated by inhibition of matriptase or MTSP1. Thus, (R)-5-[3-(diaminomethyl)phenyl]-4-[(1-formyl-(S)-4-guanidinobutylcarbamoylmethyl)carbamoyl]-4-(methoxycarbonylamino)pentanoic acid tert-Bu ester was prepd. and showed IC<sub>50</sub> < 100 nM for inhibition of matriptase activity.

IT 173656-55-8P 180312-25-8P 403669-25-0P  
403669-26-1P 403669-29-4P 403669-32-9P  
403669-33-0P 403669-34-1P 403669-37-4P  
403669-39-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptides as inhibitors of serine protease activity of matriptase or MTSP1)

L25 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:185072 HCAPLUS

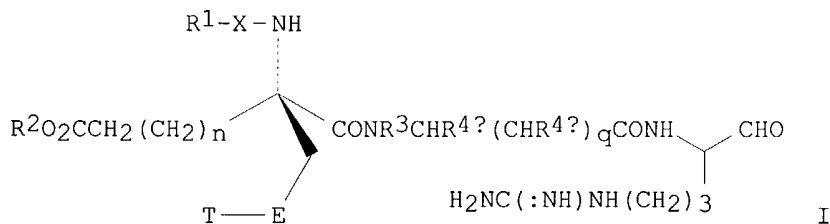
DOCUMENT NUMBER: 136:232549

TITLE: Preparation of peptides as inhibitors of serine protease activity of matriptase or MTSP1

INVENTOR(S): Duncan, David F.; Madison, Edwin L.; Semple, Joseph Edward; Coombs, Gary Samuel; Reiner, John Eugene; Ong,

PATENT ASSIGNEE(S): Edgar O.; Araldi, Gian Luca  
 SOURCE: Corvas International, Inc., USA  
 PCT Int. Appl., 82 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 4  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002020475	A2	20020314	WO 2001-US28137	20010907
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG AU 2001088922 A5 20020322 AU 2001-88922 20010907 US 2003050251 A1 20030313 US 2002-92004 20020305 PRIORITY APPLN. INFO.: US 2000-657986 A 20000908 WO 2001-US28137 W 20010907 OTHER SOURCE(S): MARPAT 136:232549 GI				



AB The invention provides compds. I [X = CO, CO<sub>2</sub>, CONH, SO<sub>2</sub>, SO<sub>2</sub>NH or a direct link; R<sub>1</sub> = (un)substituted alkyl, cycloalkyl, aryl, heterocycloalkyl, H when X is CONH, SO<sub>2</sub>, SO<sub>2</sub>NH or a direct link, etc.; R<sub>2</sub> = H, alkyl; n = 0-3; R<sub>3</sub> = H, Me; R<sub>4a</sub>, R<sub>4b</sub> = H, alkyl; q = 0-2; when q = 0, R<sub>3</sub> and R<sub>4a</sub> form prolyl or prolyl derivs., pipecolyl, or azetidine-2-carbonyl groups which are in the S-configuration; E is a 5- or 6-membered arom. ring having 0-2 ring heteroatoms; T is H, OH, CH<sub>2</sub>OH, alkyl, cyano, an amidino, guanidino, amino or carbamoyl deriv.] which inhibit serine protease activity of matriptase or MTSP1. Also provided are pharmaceutical compns. for treating conditions ameliorated by inhibition of matriptase or MTSP1. Thus, (R)-5-[3-(diaminomethyl)phenyl]-4-[(1-formyl-(S)-4-guanidinobutylcarbamoylmethyl)carbamoyl]-4-(methoxycarbonylamino)pentanoic acid tert-Bu ester was prepd. and showed IC<sub>50</sub> < 100 nM for inhibition of matriptase activity.

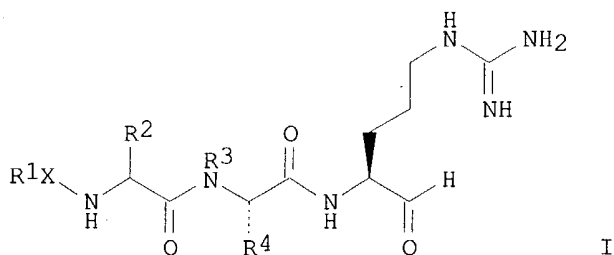
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 403669-39-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptides as inhibitors of serine protease activity of matriptase or MTSP1)

L25 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 2000:113118 HCAPLUS  
 DOCUMENT NUMBER: 132:152140  
 TITLE: Preparation of N-substituted glycine derivatives as enzyme inhibitors  
 INVENTOR(S): Abelman, Matthew Mark; Miller, Todd Anthony; Nutt, Ruth Foelsche  
 PATENT ASSIGNEE(S): Corvas International, Inc., USA  
 SOURCE: U.S., 67 pp., Cont.-in-part of U.S. 5,696,231.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6025472	A	20000215	US 1995-484509	19950607
US 5696231	A	19971209	US 1994-361794	19941221
CA 2207373	AA	19960627	CA 1995-2207373	19951221
WO 9619493	A1	19960627	WO 1995-US16866	19951221
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
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AU 716995	B2	20000316		
EP 801654	A1	19971022	EP 1995-944234	19951221
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV				
BR 9510264	A	19971104	BR 1995-10264	19951221
CN 1171116	A	19980121	CN 1995-196925	19951221
HU 77524	A2	19980528	HU 1998-71	19951221
JP 10512550	T2	19981202	JP 1995-520031	19951221
NZ 300829	A	20010330	NZ 1995-300829	19951221
PRIORITY APPLN. INFO.:			US 1994-361794	A2 19941221
			US 1995-484509	A 19950607
			WO 1995-US16866	W 19951221
OTHER SOURCE(S):		MARPAT 132:152140		
GI				



AB Glycine derivs. I [X = SO<sub>2</sub>, NR'SO<sub>2</sub>, CO, O<sub>2</sub>C, NHCO, P(O)R'', bond; R' = H, alkyl, aryl, aralkyl; R'' = NR', OR', R', SR'; R<sub>1</sub> = H, substituted benzyl or naphthyl; R<sub>2</sub> = H, tetrazol-5-ylalkyl, tetrazol-5-ylalkylsulfonylmethyl,

pyridin-3-ylalkyl, H, 3-guanidinopropyl, 2-methylsulfonylethyl, etc.; R3 = H, cycloalkyl, (un)substituted alkyl or aryl; R4 = H, (un)substituted alkyl or aryl] were prepd. as potent inhibitors of factor Xa. Thus, D-camphorsulfonyl-D-arginine-sarcosine-arginine aldehyde, prepd. by soln. phase methods, inhibited factor Xa catalytic activity with IC50 = 8.2 nM.

IT 180312-25-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of N-substituted glycine derivs. as enzyme inhibitors)

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:30818 HCAPLUS

DOCUMENT NUMBER: 132:231498

TITLE: Design, synthesis and structure-activity relationship of a series of arginine aldehyde factor Xa inhibitors. Part 1: Structures based on the (D)-Arg-Gly-Arg tripeptide sequence

AUTHOR(S): Marlowe, Charles K.; Sinha, Uma; Gunn, Alice C.; Scarborough, Robert M.

CORPORATE SOURCE: COR Therapeutics, Inc., South San Francisco, CA, 94080, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2000), 10(1), 13-16

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of arginine aldehyde inhibitors was designed as transition state (TS) analogs based on the known factor Xa specific substrate Cbz-D-Arg-Gly-Arg-pNA. BnSO2-(D)Arg-Gly-Arg-H was found to be the most potent and selective inhibitor of factor Xa and prothrombinase activity in this series.

IT 180312-25-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PNU (Preparation, unclassified); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(design, synthesis and SAR of arginine aldehyde factor Xa inhibitors based on the Arg-Gly-Arg tripeptide sequence)

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1997:701469 HCAPLUS

DOCUMENT NUMBER: 127:346661

TITLE: Preparation of methionine sulfone and S-substituted cysteine sulfone derivatives as enzyme inhibitors

INVENTOR(S): Abelman, Matthew M.; Ardecky, Robert J.; Nutt, Ruth F.

PATENT ASSIGNEE(S): Corvas International, Inc., USA

SOURCE: U.S., 82 pp., Cont.-in-part of U.S. Ser. No. 229,298. CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5681844	A	19971028	US 1994-234811	19940428
US 5776927	A	19980707	US 1994-229298	19940418
WO 9528420	A1	19951026	WO 1995-US4954	19950418

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RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

AU 9523609 A1 19951110 AU 1995-23609 19950418

EP 765340 A1 19970402 EP 1995-917624 19950418

EP 765340 B1 20000830

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE

US 5658939 A 19970819 US 1995-423584 19950418

JP 09512022 T2 19971202 JP 1995-527181 19950418

AT 195947 E 20000915 AT 1995-917624 19950418

US 5646165 A 19970708 US 1995-485826 19950606

US 5770600 A 19980623 US 1995-473647 19950606

PRIORITY APPLN. INFO.:

US 1994-229298 A2 19940418

US 1994-234811 A 19940428

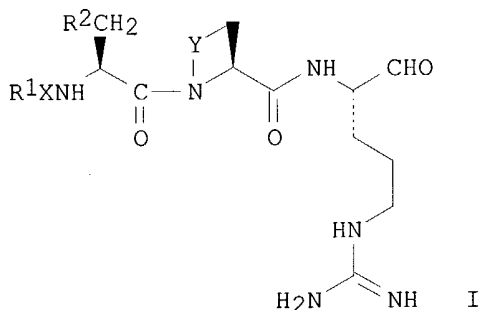
US 1995-423584 A1 19950418

WO 1995-US4954 W 19950418

OTHER SOURCE(S):

MARPAT 127:346661

GI



AB Enzyme inhibitory title compds. I [X = CO, SO<sub>2</sub>, OSO<sub>2</sub>, NHSO<sub>2</sub>, alkyl-, aryl-, or aralkyliminosulfonyl; R<sub>1</sub> = (un)substituted alkyl, alkenyl, aryl, aralkyl, or aralkenyl or perfluoroalkyl, perfluoroaryl, trimethylsilylalkyl; R<sub>2</sub> = MeSCH<sub>2</sub>, MeSOCH<sub>2</sub>, MeSO<sub>2</sub>CH<sub>2</sub> or derivs. from substitution at Me; Y = (CH<sub>2</sub>)<sub>n</sub>, where n = 1, 2, 3] or their pharmaceutically acceptable salts were prepd. Thus, N-(butanesulfonyl)-L-methioninesulfone-L-proline-L-argininal, prepd. via solid-phase reaction of N-(butanesulfonyl)-L-methioninesulfone-L-proline, showed IC<sub>50</sub> values of 0.0016 and 0.199 .mu.M for inhibition of thrombin and plasmin, resp.

IT 173534-53-7P 173656-55-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of methionine sulfone and S-substituted cysteine sulfone derivs. as enzyme inhibitors)

L25 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1997:574514 HCAPLUS

DOCUMENT NUMBER: 127:220992

TITLE: Preparation of methionine sulfone and S-substituted cysteine sulfone derivatives as thrombin or factor Xa inhibitors

INVENTOR(S): Abelman, Matthew Mark; Ardecky, Robert John; Nutt, Ruth Foelsche

PATENT ASSIGNEE(S): Corvas International Inc., USA

SOURCE: U.S., 88 pp., Cont.-in-part of U.S. Ser. No. 234,811,  
abandoned.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 3  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5658939	A	19970819	US 1995-423584	19950418
US 5776927	A	19980707	US 1994-229298	19940418
US 5681844	A	19971028	US 1994-234811	19940428
US 5770600	A	19980623	US 1995-473647	19950606

PRIORITY APPLN. INFO.: US 1994-229298 A2 19940418  
US 1994-234811 A2 19940428  
US 1995-423584 A1 19950418

OTHER SOURCE(S): MARPAT 127:220992  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. I [ R1 = alkyl, alkenyl, (substituted) aryl, heterocyclyl  
such as indole, etc.; X = CO, O2C, NHCO, SO2, O3S, NHSO2, etc.; R2 =  
CH2S(O)q(CH2)mZ where q = 0-2, m = 1-6 and Z = H, (substituted) CO2H,  
(substituted) CONH2; Y = (CH2)n where n = 1-3] were prepd. as thrombin or  
factor Xa inhibitors. Methionine sulfone II was prepd. from the  
resin-bound semicarbazone III (R = MBHA resin); III was coupled with  
Boc-Pro-OH and N-cyclohexylmethanesulfonyl-L-methionine sulfone,  
successively, followed by cleavage of the protected semicarbazone from the  
resin and hydrolysis of the semicarbazone to give II. II exhibited IC50  
values of 0.00066 and 0.030 .mu.M against thrombin and plasmin, resp.

IT 173656-55-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);  
BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of peptide aldehydes contg. methionine or cysteine sulfones as  
thrombin, factor Xa or plasmin inhibitors)

L25 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1996:527345 HCAPLUS  
DOCUMENT NUMBER: 125:196382  
TITLE: Preparation of peptide aldehydes as inhibitors of  
factor Xa.  
INVENTOR(S): Abelman, Matthew Mark; Miller, Todd Anthony; Nutt,  
Ruth Foelsche  
PATENT ASSIGNEE(S): Corvas International, Inc., USA  
SOURCE: PCT Int. Appl., 76 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9619493	A1	19960627	WO 1995-US16866	19951221

W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI,  
GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD,  
MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ,

TM, TT

RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

US 5696231	A	19971209	US 1994-361794	19941221
US 6025472	A	20000215	US 1995-484509	19950607
AU 9646086	A1	19960710	AU 1996-46086	19951221
AU 716995	B2	20000316		
EP 801654	A1	19971022	EP 1995-944234	19951221

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV

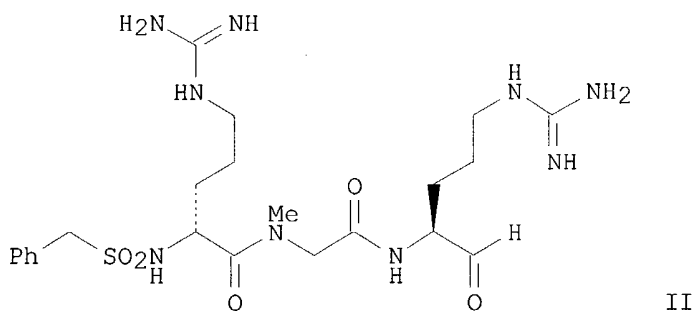
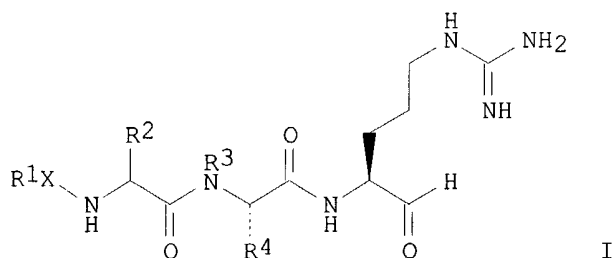
BR 9510264	A	19971104	BR 1995-10264	19951221
JP 10512550	T2	19981202	JP 1995-520031	19951221
NZ 300829	A	20010330	NZ 1995-300829	19951221

PRIORITY APPLN. INFO.:

US 1994-361794	A	19941221
US 1995-484509	A	19950607
WO 1995-US16866	W	19951221

OTHER SOURCE(S): MARPAT 125:196382

GI



AB Title compds. [I; X = SO<sub>2</sub>, NR'SO<sub>2</sub>, CO, O<sub>2</sub>C, NHCO, P(O)R'', bond; R' = H, alkyl, aryl, aralkyl; R'' = NR', OR', R', SR'; R<sub>1</sub> = H, (substituted) alkyl, cycloalkyl, heterocycloalkyl, heterocyclyl, alkenyl, aryl, heteroaryl, aralkyl, aralkenyl, CHF<sub>2</sub>, perfluoroalkyl, perfluoroaryl, etc.; R<sub>2</sub> = H, tetrazol-5-ylalkyl, tetrazol-5-ylalkylsulfonylmethyl, pyridin-3-ylalkyl, guanidinoalkyl, methylsulfonylalkyl, etc.; R<sub>3</sub> = H, (substituted) alkyl, cycloalkyl, aryl; R<sub>4</sub> = H, (substituted) alkyl; with provisos], were prepd. Thus, title compd. (II), prepd. by soln. phase methods, inhibited factor Xa catalytic activity with IC<sub>50</sub> = 1.7 nM.

IT **180312-25-8P 180313-16-0P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of peptide aldehydes as inhibitors of factor Xa)



L25 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1995:998134 HCAPLUS

DOCUMENT NUMBER: 124:176949

TITLE: Preparation of methionine sulfone and S-substituted cysteine sulfone derivatives as inhibitors of thrombin or Factor Xa.

INVENTOR(S): Abelman, Matthew M.; Ardecky, Robert John; Nutt, Ruth Foelsche

PATENT ASSIGNEE(S): Corvas International, Inc., USA

SOURCE: PCT Int. Appl., 245 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9528420	A1	19951026	WO 1995-US4954	19950418
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5776927	A	19980707	US 1994-229298	19940418
US 5681844	A	19971028	US 1994-234811	19940428
AU 9523609	A1	19951110	AU 1995-23609	19950418
EP 765340	A1	19970402	EP 1995-917624	19950418
EP 765340	B1	20000830		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 09512022	T2	19971202	JP 1995-527181	19950418
AT 195947	E	20000915	AT 1995-917624	19950418
PRIORITY APPLN. INFO.:			US 1994-229298	A 19940418
			US 1994-234811	A 19940428
			WO 1995-US4954	W 19950418
OTHER SOURCE(S):		MARPAT 124:176949		
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. [I; X = CO, O<sub>2</sub>C, NHCO, SO<sub>2</sub>, OSO<sub>2</sub>, NRSO<sub>2</sub>; R = alkyl, aryl, aralkyl; R<sub>1</sub> = alkyl, cycloalkylalkyl, alkenyl, cycloalkylalkenyl, perfluoroalkyl, perfluoroaryl, trimethylsilylalkyl, (substituted) aryl, aralkyl, aralkenyl, etc.; R<sub>2</sub> = CH<sub>2</sub>SO<sub>2</sub>Me, CH<sub>2</sub>SO<sub>2</sub>(CH<sub>2</sub>)<sub>m</sub>CO<sub>2</sub>H, CH<sub>2</sub>SO<sub>2</sub>(CH<sub>2</sub>)<sub>m</sub>CO<sub>2</sub>R, etc.; m = 1-6; n = 1-3; q = 0-2], were prepd. for preventing thrombosis. Thus, title compd. (II) inhibited FeCl<sub>3</sub>-induced thrombosis in rats with ED<sub>50</sub> = 0.7 mg/kg.

IT 173534-53-7P 173656-55-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of methionine sulfone and S-substituted cysteine sulfone derivs. as inhibitors of thrombin or Factor Xa)

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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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FILE COVERS 1907-1966  
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

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FILE 'REGISTRY' ENTERED AT 10:05:11 ON 19 MAR 2003  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 18 MAR 2003 HIGHEST RN 499968-86-4  
DICTIONARY FILE UPDATES: 18 MAR 2003 HIGHEST RN 499968-86-4

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

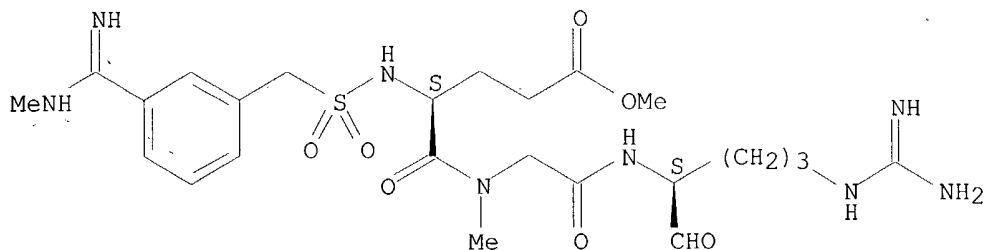
Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> d ide can l24 tot

L24 ANSWER 1 OF 12 REGISTRY COPYRIGHT 2003 ACS  
RN 403669-39-6 REGISTRY  
CN Glycinamide, N-[[[3-[imino(methylamino)methyl]phenyl]methylsulfonyl]-L-.alpha.-glutamyl-N-[(1S)-4-[(aminoiminomethyl)amino]-1-formylbutyl]-N2-methyl-, methyl ester (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C24 H38 N8 O7 S  
SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)

2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:232549

L24 ANSWER 2 OF 12 REGISTRY COPYRIGHT 2003 ACS

RN 403669-37-4 REGISTRY

CN 1H-Tetrazole-5-butanamide, N-[2-[[[(1S)-4-[(aminoiminomethyl)amino]-1-formylbutyl]amino]-2-oxoethyl]-.alpha.-[[[3-(aminoiminomethyl)phenyl]methyl]sulfonyl]amino]-N-methyl- (9CI) (CA INDEX NAME)

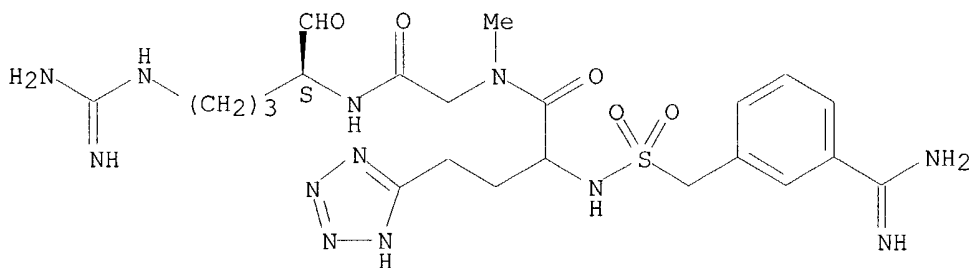
FS STEREOSEARCH

MF C22 H34 N12 O5 S

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)

2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:232549

L24 ANSWER 3 OF 12 REGISTRY COPYRIGHT 2003 ACS

RN 403669-34-1 REGISTRY

CN Butanamide, N-[(1S)-2-[[[(1S)-4-[(aminoiminomethyl)amino]-1-formylbutyl]amino]-1-methyl-2-oxoethyl]-2-[(phenylsulfonyl)amino]-, (2R)- (9CI) (CA INDEX NAME)

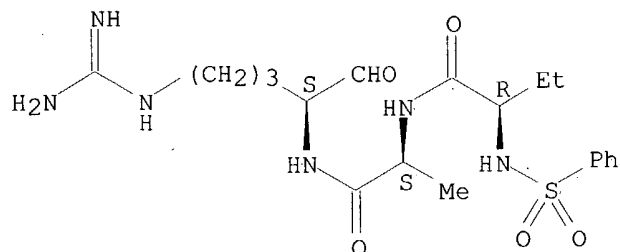
FS STEREOSEARCH

MF C19 H30 N6 O5 S

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



#13

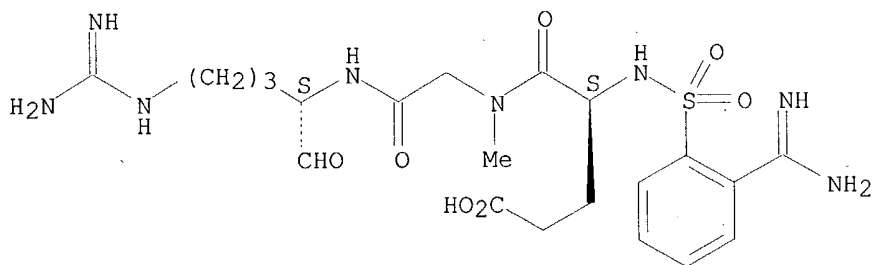
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:232549

L24 ANSWER 4 OF 12 REGISTRY COPYRIGHT 2003 ACS  
RN 403669-33-0 REGISTRY  
CN Glycinamide, N-[[2-(aminoiminomethyl)phenyl]sulfonyl]-L-.alpha.-glutamyl-N-  
[(1S)-4-[(aminoiminomethyl)amino]-1-formylbutyl]-N2-methyl- (9CI) (CA  
INDEX NAME)  
FS STEREOSEARCH  
MF C21 H32 N8 O7 S  
SR CA  
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



#12

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

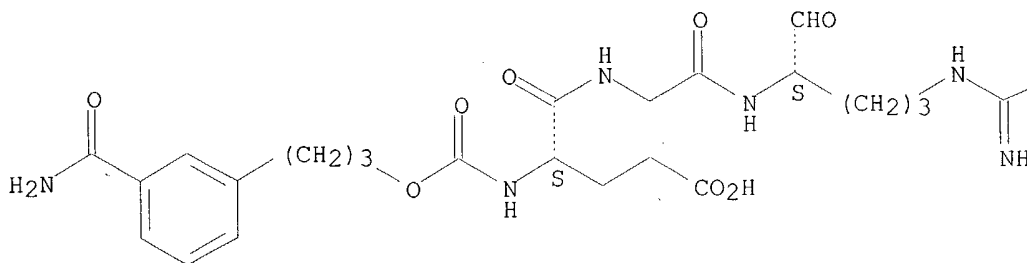
REFERENCE 1: 136:232549

L24 ANSWER 5 OF 12 REGISTRY COPYRIGHT 2003 ACS  
RN 403669-32-9 REGISTRY  
CN Glycinamide, N-[[3-[3-(aminocarbonyl)phenyl]propoxy]carbonyl]-L-.alpha.-  
glutamyl-N-[(1S)-4-[(aminoiminomethyl)amino]-1-formylbutyl]- (9CI) (CA  
INDEX NAME)  
FS STEREOSEARCH  
MF C24 H35 N7 O8  
SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

NH2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)

2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:232549

L24 ANSWER 6 OF 12 REGISTRY COPYRIGHT 2003 ACS

RN 403669-29-4 REGISTRY

CN Glycinamide, N-[[[4-(aminocarbonyl)phenyl]methyl]sulfonyl]-L-.alpha.-glutamyl-N-[(1S)-4-[(aminoiminomethyl)amino]-1-formylbutyl]-N2-methyl-(9CI) (CA INDEX NAME)

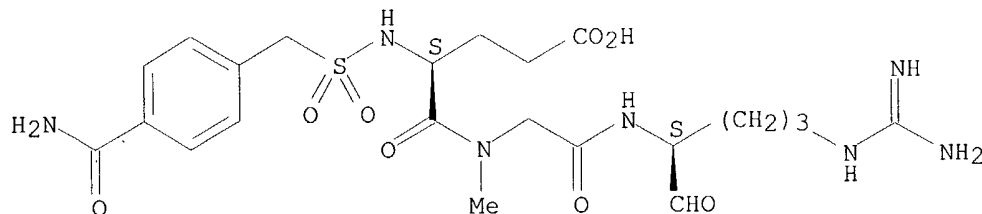
FS STEREOSEARCH

MF C22 H33 N7 O8 S

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

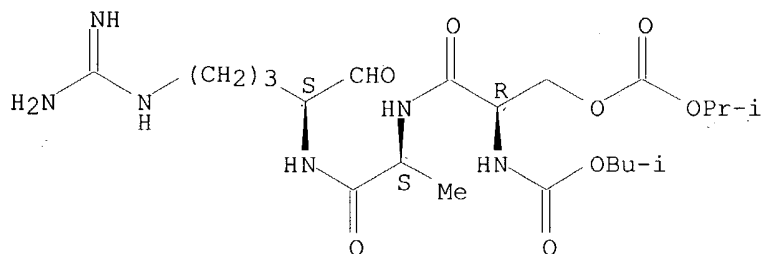
1 REFERENCES IN FILE CA (1962 TO DATE)

2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:232549

L24 ANSWER 7 OF 12 REGISTRY COPYRIGHT 2003 ACS  
 RN 403669-26-1 REGISTRY  
 CN L-Alaninamide, O-[(1-methylethoxy)carbonyl]-N-[(2-methylpropoxy)carbonyl]-  
 D-seryl-N-[(1S)-4-[(aminoiminomethyl)amino]-1-formylbutyl]- (9CI) (CA  
 INDEX NAME)  
 FS STEREOSEARCH  
 MF C21 H38 N6 O8  
 SR CA  
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.



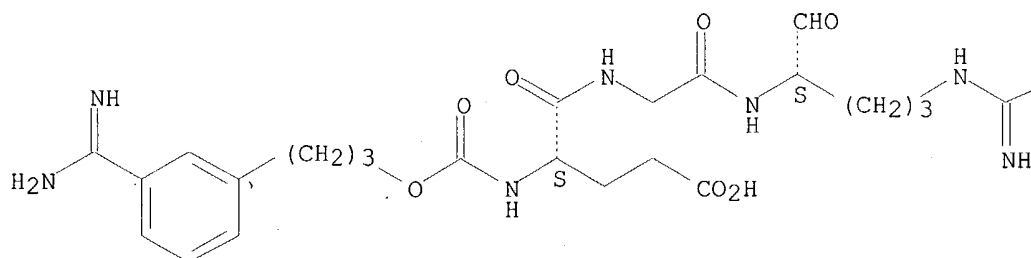
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
 2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:232549

L24 ANSWER 8 OF 12 REGISTRY COPYRIGHT 2003 ACS  
 RN 403669-25-0 REGISTRY  
 CN Glycinamide, N-[[3-[3-(aminoiminomethyl)phenyl]propoxy]carbonyl]-L-.alpha.-  
 glutamyl-N-[(1S)-4-[(aminoiminomethyl)amino]-1-formylbutyl]- (9CI) (CA  
 INDEX NAME)  
 FS STEREOSEARCH  
 MF C24 H36 N8 O7  
 SR CA  
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PAGE 1-A

PAGE 1-B

NH2

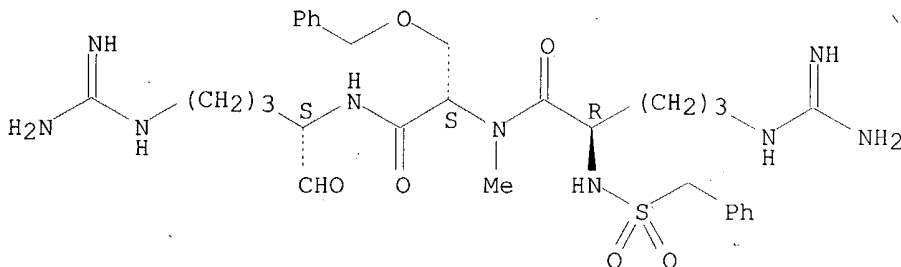
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2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:232549 *Sur 44*

L24 ANSWER 9 OF 12 REGISTRY COPYRIGHT 2003 ACS  
RN 180313-16-0 REGISTRY  
CN L-Serinamide, N2-[(phenylmethyl)sulfonyl]-D-arginyl-N-[4-  
[(aminoiminomethyl)amino]-1-formylbutyl]-N2-methyl-O-(phenylmethyl)-, (S)-  
(9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C30 H45 N9 O6 S  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



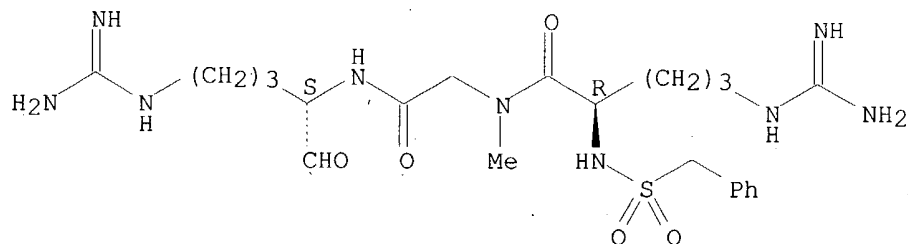
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:196382

L24 ANSWER 10 OF 12 REGISTRY COPYRIGHT 2003 ACS  
RN 180312-25-8 REGISTRY  
CN Glycinamide, N2-[(phenylmethyl)sulfonyl]-D-arginyl-N-[(1S)-4-  
[(aminoiminomethyl)amino]-1-formylbutyl]-N2-methyl- (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN Glycinamide, N2-[(phenylmethyl)sulfonyl]-D-arginyl-N-[4-  
[(aminoiminomethyl)amino]-1-formylbutyl]-N2-methyl-, (S)-  
FS STEREOSEARCH  
MF C22 H37 N9 O5 S  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



#17

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1962 TO DATE)  
5 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:232549  
REFERENCE 2: 132:231498  
REFERENCE 3: 132:152140  
REFERENCE 4: 125:196382

inst ↑

L24 ANSWER 11 OF 12 REGISTRY COPYRIGHT 2003 ACS

RN 173656-55-8 REGISTRY

CN L-Prolinamide, (2S)-2-[[[(7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl)methyl]sulfonyl]amino]-4-(methylsulfonyl)butanoyl-N-[(1S)-4-[(aminoiminomethyl)amino]-1-formylbutyl]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN L-Prolinamide, N-[[[(7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl)methyl]sulfonyl]-4-(methylsulfonyl)-L-2-aminobutanoyl-N-[4-[(aminoiminomethyl)amino]-1-formylbutyl]-, [1(1S),2(S)]-

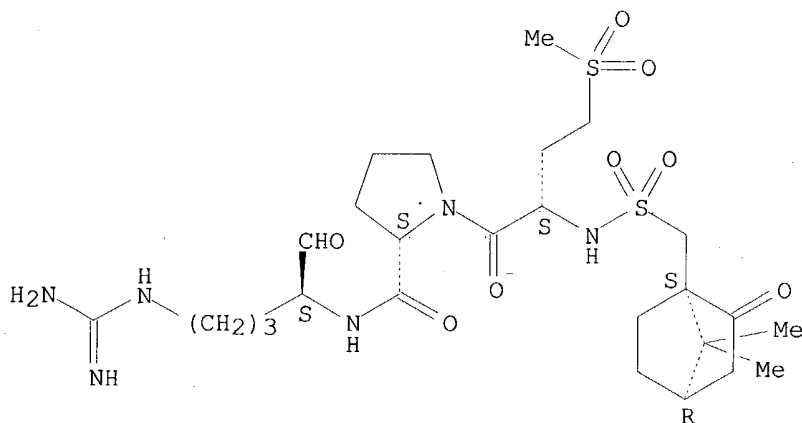
FS STEREOSEARCH

MF C26 H44 N6 O8 S2

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



#15

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

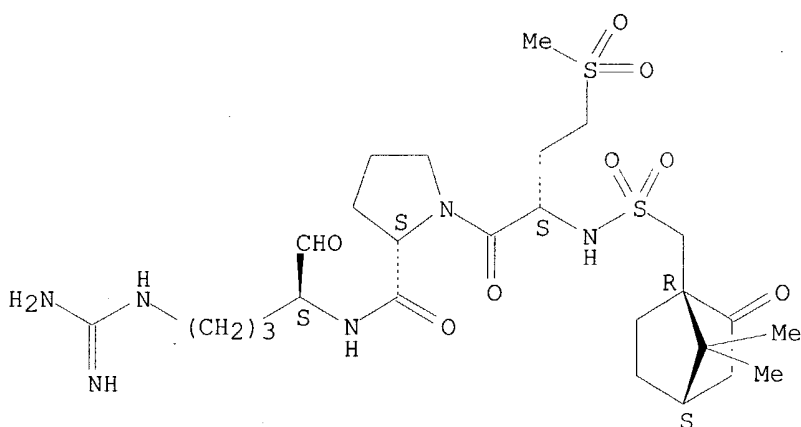


4 REFERENCES IN FILE CA (1962 TO DATE)  
5 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:232549  
REFERENCE 2: 127:346661  
REFERENCE 3: 127:220992  
REFERENCE 4: 124:176949

L24 ANSWER 12 OF 12 REGISTRY COPYRIGHT 2003 ACS  
RN 173534-53-7 REGISTRY  
CN L-Prolinamide, N-[[[(7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl)methyl]sulfonyl]-4-(methylsulfonyl)-L-2-aminobutanoyl-N-[4-[(aminoiminomethyl)amino]-1-formylbutyl]-, [1(1R),2(S)]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C26 H44 N6 O8 S2  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1962 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 127:346661  
REFERENCE 2: 124:176949